

Perfluoroheptanoic acid  
375-85-9 | DTXSID1037303

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.58

Global applicability domain: Inside

Local applicability domain index: 4.21e-01

Confidence level: 3.96e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctan-1-ol</div> <div>Measured: 4.54</div> <div>Predicted: 4.45</div>	<div>Image not found</div> <div>Perflenapent</div> <div>Measured: 4.40</div> <div>Predicted: 4.23</div>	<div>Image not found</div> <div>1,1,2,2-Tetrahydroperfluoro-1-decanol</div> <div>Measured: 5.58</div> <div>Predicted: 5.05</div>
<div>Image not found</div> <div>1-Decyl-2,4-dimethylpyridin-1-ium iodide</div> <div>Measured: 0.54</div> <div>Predicted: 4.75</div>	<div>Image not found</div> <div>1-Dodecyl-2-methylpyridin-1-ium iodide</div> <div>Measured: 1.32</div> <div>Predicted: 4.22</div>	